A Control Strategy for Extractive and Reactive Divided Wall Columns

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1. Introduction

As a thermal separation method, distillation is one of the most important separation technologies in the chemical industry. Basically, in every production process sorne of the chemicals go through at least one distillation column on their way from raw species to final product. Distillation is and will remain the separation method of choice in the chemical industry (there are more than 50.000 columns in operation around the world). Despite its flexibility and widespread use, this unit operation is very energy demanding, which constitutes one important drawback. Distillation can generate more than 50% of plant operating costs and it is the responsible of 3% of the energy usage in the US (notice that the thermodynamic efficiency of a distillation column is between 5-20%). In order to reduce this drawback new approaches and configurations have appeared.

Conventional temary separations progressed via thermally coupled columns such as Petlyuk configuration to a novel design that integrates two distillation columns into one shell setup known today as dividing-wall column (DWC). The DWC concept is a major breakthrough in distillation technology, as both energy consumption and capital cost can be reduced. In fact, using dividing-wall columns can save up to 30% in the capital invested and up to 40% in the energy costs particularly for close boiling species. Several companies like Montz, BASF or AzkoNobel are actively researching in this area (Kiss 2012, Bravo-Bravo 2010). However, the control of a divided-wall column is more difficult than the control of a conventional schema with two columns for the separation of temary mixtures because there is more interaction among control loops.

Sorne recent work has been presented extending DWC to other distillation setups, like extractive DWC and reactive DWC with important industrial applications like using extractive DWC for bioethanol dehydration. Sorne work has been done related to have a good control structure for conventional DWC (van Diggelen 2010, Kiss and Suszwalak 2011) or their control using multivariable predicive control (Rodriguez and Chinea 2012, Rewagad and Kiss 2012) but there are very few works addressing the control of reactive and extractive DWC. In this work we present the control of extractive and reactive divided wall columns using a decentralized approach as well as using the multivariable predictive controller approach.

The remaining of the paper is organised as follows. Section two describes the methodology. Section three simulates and designs the decentralized control structure and the MPC for the extractive DWC. Section four presents the reactive DWC case study along with its simulation and model predictive control. Finally, section five draws conclusions and discusses the obtained results.

2. Methodology

The methodology explained in this section has been applied to the extractive and reactive divided wall columns case studies. First of all a steady state simulation of the thermodinamically equivalent configuration was developed. This model was used to size the equipments and create the dynamic simulation (Aspen Plus and Aspen Dynamics have been used for these two tasks). The decentralized control has been implemented in the dynamic simulator. To generate the model for the MPC an API has been used called Control Design Interface. This API generates the linearized state space model. This model has been scaled in order to avoid very different magnitudes and implemented in Matlab. Before using the generated model for the MPC a validation has been performed. In order to validate the model, a simulink wrapper of the original dynamic simulation is developed. Using the Simulink environment the linear model is validated against the rigorous one. Figure 1 shows the explained procedure.

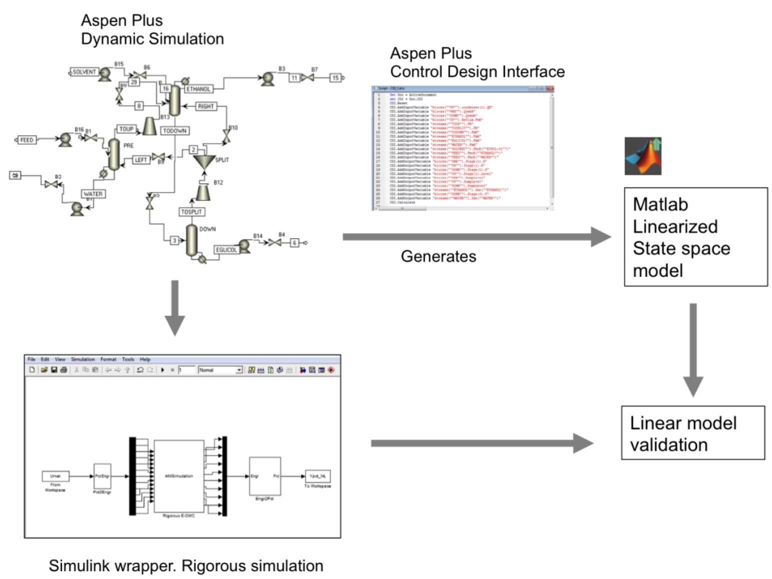

Figure 1: Methodology to generate the model for the MPC

Once the state space model is available the MPC is designed (in Simulink). Figure 2 shows the final structure. The model predicitive controller is connected to the rigorous model (thorough the Simulink wrapper *AMSimulation* block). The *Pct2Eng* and *Eng2Pct* blocks are unit converters from engineering to percentege, this is necessary as the MPC is scaled. The MPC parameters are tuned (control and prediction horizons, sampling time, weighting factors for the controlled variables) and the final MPC is used to evaluate its performance under different disturbances.

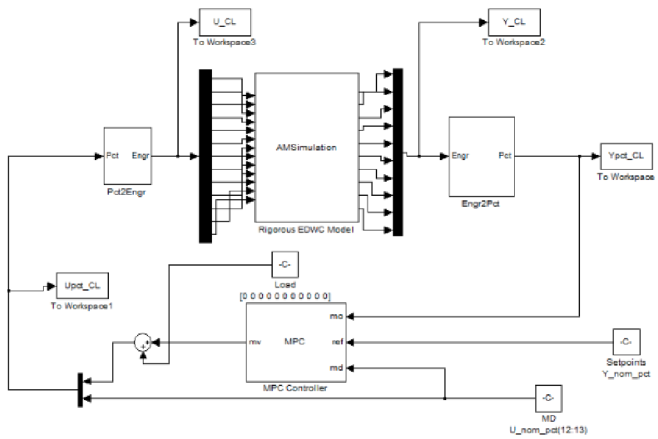

Figure 2: MPC configuration in Simulink

3. Extractive Divided Wall Columns Case Study

The case study is based on the paper by Kiss and Ignat (2012) where they present the use of an extractive dividing-wall column for bioethanol dehydration. The ethanol dehydration and concentration is achieved using ethylene glycol as the extracting agent. The feed is a mixture with 10%w ethanol. Figure 3 shows the extractive DWC setup as well as its thermodinamically equivalent configuration with conventional columns. In this particular configuration the liquid back from the upper part of the wall only goes to the right part of the wall. This last configuration has been simulated with Aspen Plus and has been used to design the decentralized control and to generate the model to be used for the Model Predictive Control. The decentralized control implemented is shown in the figure.

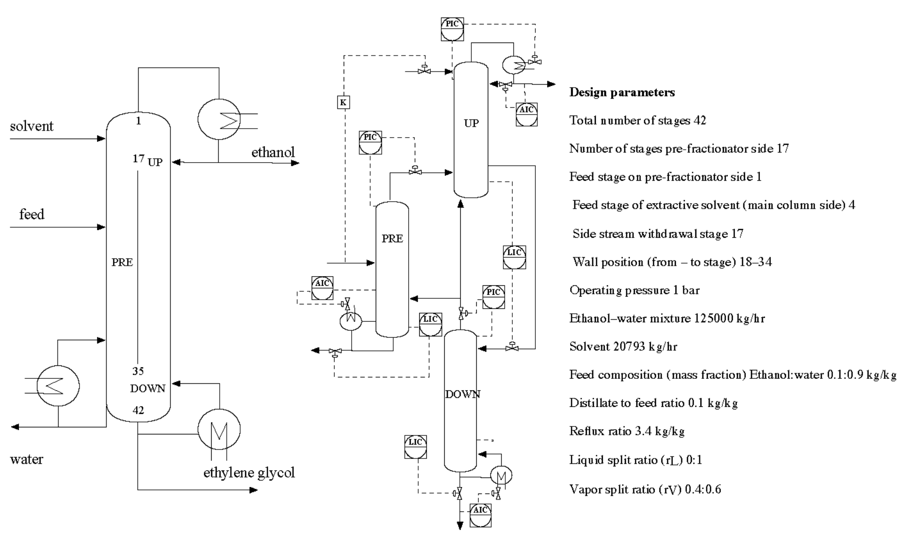

Figure 3: Extractive DWC and its thermodinamically equivalent configuration implemented for control design

The controlled variables in the simulation are: levels, compositions and pressures. It is important to notice that there are some additional controls that are not in the actual extractive DWC but they are neccessary for the simulation. Figure 4 shows the results of the decentralized control. Water and ethanol compositions and column pressure and bottoms level are shown. The obtained response corresponds to a 2.5% disturbance in the feed. Although the disturbances are compensanted the system exhibits a oscillatory response, there is strong interaction between control loops which makes decentralized control very difficult. A lot of effort has to be put into tunning parameters to improve the response and make it less oscillatory.

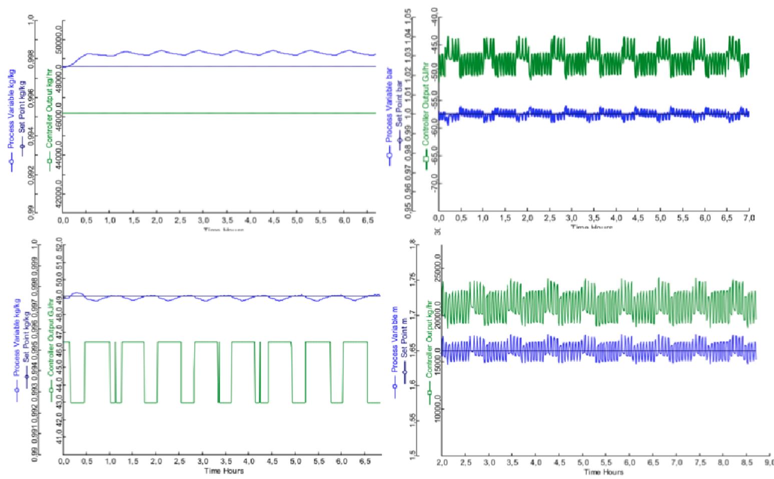

Figure 4: Decentralized control: up left ethanol composition, down left water composition, up right pressure, down right level

Results for the MPC configuration are shown in Figure 5. The same 2.5% feed flow disturbance has been applied. The figure includes the ethylene glycol composition which is controlled by inference with the temperature of a sensitive tray. The control achieves a smooth response and with a good performance. Higher disturbances have been tested with a positive response by the MPC controller. The controller includes constraints for the manipulated and controlled variables in order to avoid great step changes for the manipulated variables or unfeasible situations (compositions greater than 1, levels above 100% and so on). The prediction horizon is set to 20 and the control horizon to 4, the sampling time is 2 minutes.

4. Reactive Divided Wall Columns Case Study

The case study is based on the paper by Sander et al., 2007 where they present the use of a reactive dividing-wall column for the hydrolysis of Methyl Acetate to produce Methanol and Acetic Acid. This system has been widely studied to illustrate reactive distillation columns as it reduces drastically the number of columns regarding the original process. A reactive divided wall column was studied in that work as an improvement to the reactive distillation. In this case Figure 6 shows the reactive DWC setup as well as its thermodinamically equivalent configuration with conventional columns. The reactive DWC has 63 stages, the wall starts in stage 10 and it continues until stage 52. The left part of the wall is simulated as a reactive column being the reactive zone between stages 6 and 17. Water is fed pure and Methyl acetate is fed with 19%w of methanol. Water is set to have a mole ratio of three to Methyl acetate.

The model predictive controller has been developed and implemented for this system following the described methodology. The prediction horizon is set to 20 and the control horizon to 4, the

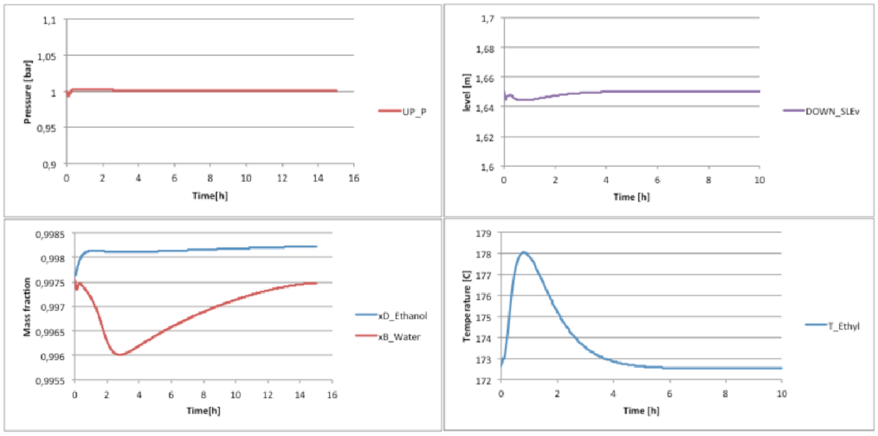

Figure 5: MPC control: up left pressure, down left water and ethanol composition, up right level, down right ethylene glycol composition (temperature inference)

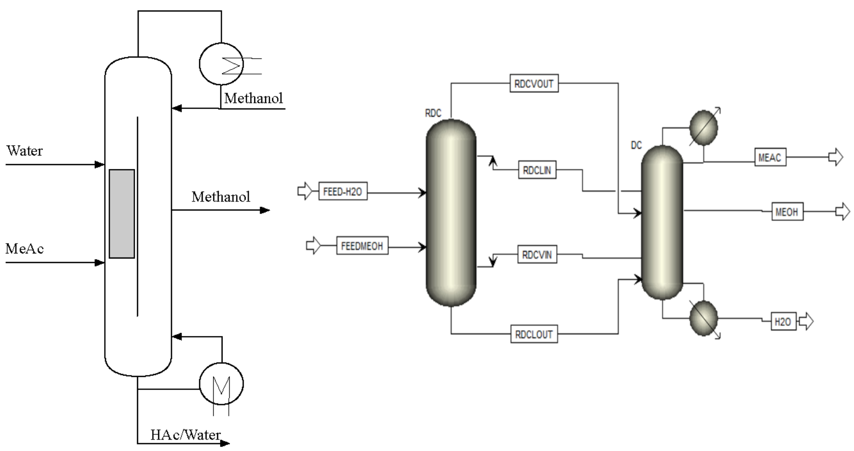

Figure 6: Reactive DWC and its thermodinamically equivalent configuration implemented for control design

sampling time is 2 minutes. In Figure 7 the controller response is shown. Left figure represents the composition control for the three outputs of the RDWC, right figure shows the pressure and level control (up and down figures respectively). As it can be observed the disturbances are handled without any difficulties by the MPC. The controller has shown a more robust behaviour than with the extractive DWC handling higher disturbances without problems.

5. Conclusions

Divinding-wall columns are a promising alternative for some processes but these are complex, very integrated units with strong interactions. Extractive and reactive divided wall columns are still more complex operations and its control is a difficult task. In the case of the extractive divided wall columns the decentralized as well as the multivariable predictive control have been implemented. The decentralized control shows a very oscillatory response as the result of the interactions being difficult to control, on the other hand the MPC shows a smooth response and good control being able to handle larger disturbances than the decentralized option. In the case of

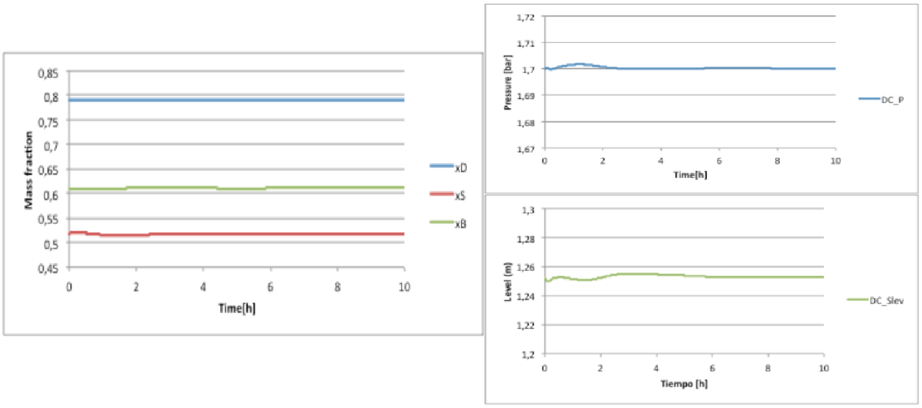

Figure 7: MPC results for a 5% feed disturbance: left figure shows compositon control, up right pressure control and down right level control

the reactive divided wall column just the MPC results are presented. It also shows a good control performance. It behaves even better than the MPC of the extractive DWC, handling better larger disturbances. This work is being completed with the analysis of azeotropic divided wall columns and it will be presented somewhere in a near future along with the MPC for DWC, E-DWC and R-DWC.